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Shuja, Shaukat; Ali, Saqib; Meetsma, Auke; Broker, Grant A.; Tiekink, Edward R. T.

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Shaukat Shuja,^a Saqib Ali,^a Auke Meetsma,^b Grant A. Broker^c and Edward R. T. Tiekink^{c*}

^aDepartment of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, ^bCrystal Structure Center, Chemical Physics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands, and ^cDepartment of Chemistry, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249-0698, USA

Correspondence e-mail:
edward.tiekink@utsa.edu

Key indicators

Single-crystal X-ray study
 $T = 100\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
Disorder in main residue
 R factor = 0.046
 wR factor = 0.139
Data-to-parameter ratio = 10.5

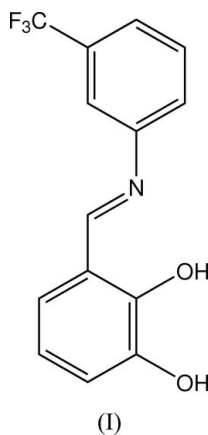
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

3-[3-(Trifluoromethyl)phenyliminomethyl]-benzene-1,2-diol

The crystal packing of the essentially planar molecules of the title compound, $\text{C}_{14}\text{H}_{10}\text{F}_3\text{NO}_2$, is stabilized by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds and possible $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ interactions.

Comment

As part of our ongoing studies (Shuja *et al.*, 2006) of the structural aspects of hydroxy Schiff bases aimed towards the development of materials with superior optical properties and biological activities, we now report the synthesis and structure of the title compound, (I) (Fig. 1).



Molecules of compound (I) are essentially planar in the crystal structure, as manifested in the $\text{C6}-\text{N1}-\text{C8}-\text{C9}$

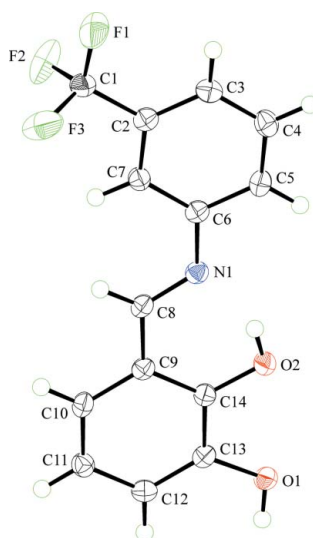
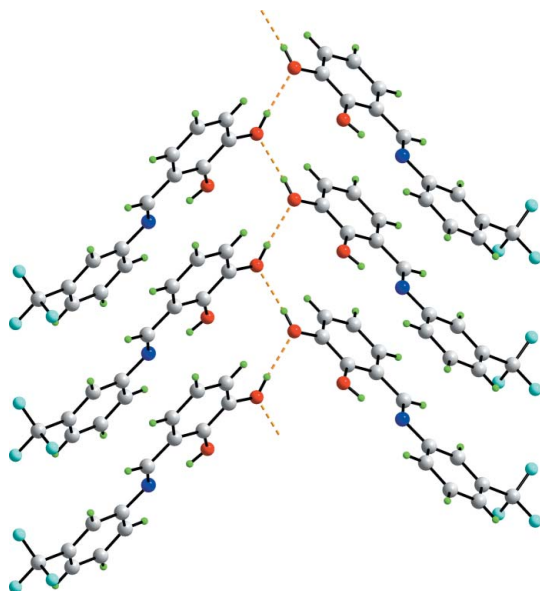


Figure 1

The molecular structure of (I), showing displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms). Only the major component of the disordered CF_3 group is shown.

**Figure 2**

Chain formation via O—H...O (orange dashed lines) interactions along the *b* axis in the structure of (I). Color code: F atoms are shown in cyan, O atoms in red, N atoms in blue, C atoms in grey and H atoms in green. Only one disorder component is shown.

torsion angle of $-179.13(14)^\circ$. Both intra- and inter-molecular O—H...O hydrogen bonds are noted in the structure (Table 1), with the latter leading to the formation of chains along the *b* axis (Fig. 2). Contacts between the chains are afforded by C—H...F interactions resulting in layers stacked along the *c* axis. The most prominent connection between layers is a C—H...O interaction.

Experimental

2,3-Dihydroxybenzaldehyde (0.5 g, 3.6 mmol) and 3-(trifluoromethyl)aniline (0.58 g, 3.6 mmol) in ethanol (40 ml) were heated under reflux for 2 h with stirring. The solution was cooled and kept in the dark. Orange–red crystals of (I) were collected after two days (m.p. 389–391 K).

Crystal data

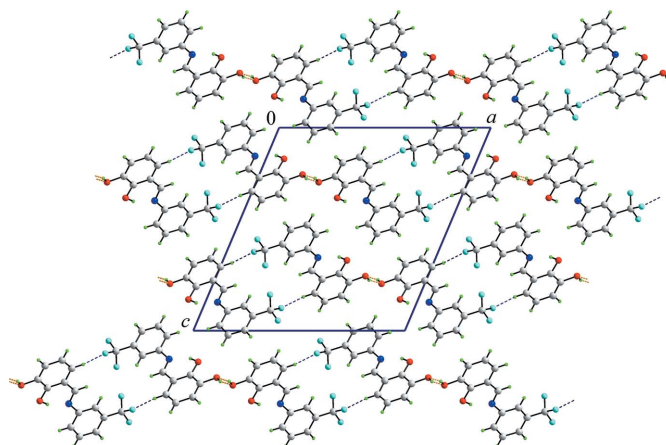
$C_{14}H_{10}F_3NO_2$	$V = 1207.92(12) \text{ \AA}^3$
$M_r = 281.23$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 16.2463(9) \text{ \AA}$	$\mu = 0.14 \text{ mm}^{-1}$
$b = 4.7716(3) \text{ \AA}$	$T = 100(2) \text{ K}$
$c = 16.9199(9) \text{ \AA}$	$0.49 \times 0.41 \times 0.22 \text{ mm}$
$\beta = 112.939(1)^\circ$	

Data collection

Bruker SMART CCD diffractometer	8910 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2006)	2109 independent reflections
$T_{\min} = 0.909$, $T_{\max} = 0.971$	1870 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$	201 parameters
$wR(F^2) = 0.139$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$
2109 reflections	$\Delta\rho_{\text{min}} = -0.40 \text{ e \AA}^{-3}$

**Figure 3**

Unit-cell contents of (I), viewed down the *c*-axis direction. Color code as for Fig. 2. The O—H...O (orange) and C—H...F (blue) interactions are shown as dashed lines. Only one disorder component is shown.

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1O\cdots O1^i$	0.84	1.93	2.7510 (15)	165
$O2-H2O\cdots N1$	0.84	1.81	2.596 (2)	154
$C10-H10\cdots F3^{ii}$	0.95	2.53	3.380 (3)	149
$C4-H4\cdots O1^{iii}$	0.95	2.61	3.392 (2)	140

Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 1, -y + 2, -z + 1$.

All H atoms were placed geometrically ($C-H = 0.95 \text{ \AA}$ and $O-H = 0.84 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ or $1.5U_{\text{eq}}(O)$. The CF_3 group is disordered over two orientations in a 0.908 (4):0.092 (4) ratio.

Data collection: SMART, (Bruker, 2006); cell refinement: SAINT-Plus (Bruker, 2006); data reduction: SAINT-Plus; program(s) used to solve structure: SIR2004 (Burla *et al.*, 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: SHELXL97.

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References

- Brandenburg, K. (2006). DIAMOND. Release 3.1. Crystal Impact GbR, Bonn, Germany.
- Bruker (2006). SMART, SAINT-Plus and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Burla, M. C., Calandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
- Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Sheldrick, G. M. (1997). SHELXL97. University of Göttingen, Germany.
- Shuja, S., Ali, S., Khalid, N., Labat, G. & Stoeckli-Evans, H. (2006). *Acta Cryst. E62*, o4786–o4788.

supporting information

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3-[3-(Trifluoromethyl)phenyliminomethyl]benzene-1,2-diol

Shaukat Shuja, Saqib Ali, Auke Meetsma, Grant A. Broker and Edward R. T. Tiekink

3-[3-(Trifluoromethyl)phenyliminomethyl]benzene-1,2-diol

Crystal data

$C_{14}H_{10}F_3NO_2$

$M_r = 281.23$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 16.2463\ (9)\ \text{\AA}$

$b = 4.7716\ (3)\ \text{\AA}$

$c = 16.9199\ (9)\ \text{\AA}$

$\beta = 112.939\ (1)^\circ$

$V = 1207.92\ (12)\ \text{\AA}^3$

$Z = 4$

$F(000) = 576$

$D_x = 1.546\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5078 reflections

$\theta = 2.6\text{--}29.5^\circ$

$\mu = 0.14\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, orange-red

$0.49 \times 0.41 \times 0.22\ \text{mm}$

Data collection

Bruker SMART CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $4096 \times 4096 / 62 \times 62$ (binned
512) pixels mm^{-1}

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2006)

$T_{\min} = 0.909$, $T_{\max} = 0.971$

8910 measured reflections

2109 independent reflections

1870 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.015$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -19 \rightarrow 17$

$k = 0 \rightarrow 5$

$l = 0 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.139$

$S = 1.06$

2109 reflections

201 parameters

8 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2 + 0.695P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.49\ \text{e}\ \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.40\ \text{e}\ \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.82417 (12)	0.3364 (4)	0.39916 (12)	0.0276 (4)	0.908 (4)
F1	0.87946 (12)	0.1499 (4)	0.45002 (11)	0.0580 (6)	0.908 (4)
F2	0.79056 (10)	0.2039 (5)	0.32209 (9)	0.0561 (6)	0.908 (4)
F3	0.87048 (13)	0.5458 (3)	0.38851 (18)	0.0816 (9)	0.908 (4)
C1A	0.82417 (12)	0.3364 (4)	0.39916 (12)	0.0276 (4)	0.092 (4)
F1A	0.8331 (15)	0.077 (2)	0.4117 (10)	0.108 (10)*	0.092 (4)
F2A	0.8099 (7)	0.389 (3)	0.3224 (6)	0.022 (4)*	0.092 (4)
F3A	0.8945 (9)	0.459 (4)	0.4482 (9)	0.062 (6)*	0.092 (4)
O1	0.29573 (8)	1.5909 (2)	0.26882 (8)	0.0247 (3)	
H1O	0.2706	1.7440	0.2496	0.037*	
O2	0.41465 (8)	1.1978 (3)	0.34631 (8)	0.0251 (3)	
H2O	0.4577	1.0850	0.3629	0.038*	
N1	0.55754 (9)	0.9236 (3)	0.35995 (9)	0.0214 (3)	
C2	0.75077 (11)	0.4256 (4)	0.42676 (11)	0.0227 (4)	
C3	0.74251 (11)	0.3013 (4)	0.49780 (11)	0.0243 (4)	
H3	0.7834	0.1607	0.5297	0.029*	
C4	0.67344 (12)	0.3867 (4)	0.52115 (11)	0.0265 (4)	
H4	0.6667	0.3036	0.5693	0.032*	
C5	0.61422 (12)	0.5926 (4)	0.47458 (11)	0.0240 (4)	
H5	0.5675	0.6501	0.4915	0.029*	
C6	0.62212 (11)	0.7168 (3)	0.40319 (11)	0.0204 (4)	
C7	0.69145 (11)	0.6307 (4)	0.37922 (11)	0.0219 (4)	
H7	0.6979	0.7120	0.3307	0.026*	
C8	0.56055 (11)	1.0658 (3)	0.29622 (11)	0.0209 (4)	
H8	0.6070	1.0300	0.2767	0.025*	
C9	0.49444 (11)	1.2791 (3)	0.25370 (11)	0.0200 (4)	
C10	0.50036 (11)	1.4337 (4)	0.18519 (11)	0.0226 (4)	
H10	0.5472	1.3949	0.1664	0.027*	
C11	0.43910 (12)	1.6407 (4)	0.14509 (11)	0.0231 (4)	
H11	0.4439	1.7443	0.0991	0.028*	
C12	0.36956 (11)	1.6977 (4)	0.17246 (11)	0.0219 (4)	
H12	0.3271	1.8397	0.1448	0.026*	
C13	0.36279 (11)	1.5480 (3)	0.23952 (11)	0.0205 (4)	
C14	0.42466 (11)	1.3369 (3)	0.28125 (11)	0.0200 (4)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0277 (9)	0.0243 (9)	0.0321 (10)	0.0041 (7)	0.0132 (8)	0.0036 (8)
F1	0.0523 (10)	0.0809 (12)	0.0511 (10)	0.0462 (9)	0.0313 (9)	0.0318 (9)

F2	0.0430 (8)	0.0863 (16)	0.0454 (9)	0.0055 (9)	0.0242 (7)	−0.0207 (8)
F3	0.0755 (13)	0.0296 (8)	0.189 (3)	−0.0035 (8)	0.1056 (16)	0.0007 (11)
C1A	0.0277 (9)	0.0243 (9)	0.0321 (10)	0.0041 (7)	0.0132 (8)	0.0036 (8)
O1	0.0219 (6)	0.0231 (6)	0.0330 (7)	0.0024 (5)	0.0150 (5)	0.0023 (5)
O2	0.0249 (6)	0.0255 (7)	0.0290 (7)	0.0042 (5)	0.0150 (5)	0.0050 (5)
N1	0.0214 (7)	0.0201 (7)	0.0229 (7)	−0.0010 (6)	0.0089 (6)	−0.0022 (6)
C2	0.0212 (8)	0.0214 (8)	0.0240 (9)	−0.0026 (7)	0.0072 (7)	−0.0037 (7)
C3	0.0234 (9)	0.0229 (9)	0.0224 (9)	−0.0001 (7)	0.0043 (7)	0.0005 (7)
C4	0.0290 (9)	0.0295 (9)	0.0202 (9)	−0.0022 (7)	0.0086 (7)	0.0010 (7)
C5	0.0232 (9)	0.0284 (9)	0.0222 (9)	−0.0022 (7)	0.0106 (7)	−0.0036 (7)
C6	0.0194 (8)	0.0192 (8)	0.0209 (8)	−0.0027 (7)	0.0060 (7)	−0.0040 (7)
C7	0.0235 (9)	0.0219 (8)	0.0212 (9)	−0.0021 (7)	0.0097 (7)	−0.0007 (7)
C8	0.0190 (8)	0.0207 (8)	0.0241 (9)	−0.0024 (7)	0.0097 (7)	−0.0046 (7)
C9	0.0191 (8)	0.0193 (8)	0.0208 (8)	−0.0025 (7)	0.0070 (7)	−0.0040 (6)
C10	0.0220 (8)	0.0249 (9)	0.0240 (9)	−0.0034 (7)	0.0123 (7)	−0.0046 (7)
C11	0.0254 (9)	0.0233 (9)	0.0206 (9)	−0.0022 (7)	0.0089 (7)	−0.0007 (7)
C12	0.0205 (8)	0.0192 (8)	0.0227 (9)	−0.0017 (7)	0.0049 (7)	−0.0023 (7)
C13	0.0173 (8)	0.0201 (8)	0.0241 (9)	−0.0031 (7)	0.0081 (7)	−0.0049 (7)
C14	0.0198 (8)	0.0191 (8)	0.0215 (8)	−0.0046 (7)	0.0087 (7)	−0.0033 (7)

Geometric parameters (Å, °)

C1—F3	1.305 (2)	C3—H3	0.9500
C1—F1	1.318 (2)	C4—C5	1.386 (3)
C1—F2	1.358 (2)	C4—H4	0.9500
C1—C2	1.502 (2)	C5—C6	1.395 (2)
C1A—F1A	1.256 (11)	C5—H5	0.9500
C1A—F2A	1.251 (9)	C6—C7	1.399 (2)
C1A—F3A	1.264 (10)	C7—H7	0.9500
C1A—C2	1.502 (2)	C8—C9	1.451 (2)
F1A—F2A	2.048 (16)	C8—H8	0.9500
O1—C13	1.377 (2)	C9—C10	1.408 (2)
O1—H1O	0.84	C9—C14	1.411 (2)
O2—C14	1.349 (2)	C10—C11	1.378 (2)
O2—H2O	0.84	C10—H10	0.9500
N1—C8	1.291 (2)	C11—C12	1.405 (2)
N1—C6	1.418 (2)	C11—H11	0.9500
C2—C3	1.393 (3)	C12—C13	1.381 (2)
C2—C7	1.389 (2)	C12—H12	0.9500
C3—C4	1.388 (3)	C13—C14	1.403 (2)
F3—C1—F1	108.92 (18)	C6—C5—H5	119.5
F3—C1—F2	105.16 (18)	C5—C6—C7	118.82 (16)
F1—C1—F2	103.26 (17)	C5—C6—N1	116.29 (15)
F3—C1—C2	113.36 (16)	C7—C6—N1	124.88 (15)
F1—C1—C2	114.21 (16)	C2—C7—C6	119.62 (16)
F2—C1—C2	111.09 (15)	C2—C7—H7	120.2
F1A—C1A—F2A	109.5 (6)	C6—C7—H7	120.2

F1A—C1A—F3A	109.3 (6)	N1—C8—C9	121.42 (15)
F2A—C1A—F3A	110.1 (5)	N1—C8—H8	119.3
F1A—C1A—C2	106.3 (10)	C9—C8—H8	119.3
F2A—C1A—C2	114.7 (5)	C10—C9—C14	119.40 (16)
F3A—C1A—C2	106.8 (7)	C10—C9—C8	120.05 (15)
C13—O1—H1O	108.8	C14—C9—C8	120.54 (15)
C14—O2—H2O	103.9	C11—C10—C9	120.83 (16)
C8—N1—C6	122.38 (15)	C11—C10—H10	119.6
C3—C2—C7	121.41 (16)	C9—C10—H10	119.6
C3—C2—C1A	120.20 (16)	C10—C11—C12	119.73 (16)
C7—C2—C1A	118.38 (16)	C10—C11—H11	120.1
C3—C2—C1	120.20 (16)	C12—C11—H11	120.1
C7—C2—C1	118.38 (16)	C13—C12—C11	120.16 (16)
C4—C3—C2	118.76 (16)	C13—C12—H12	119.9
C4—C3—H3	120.6	C11—C12—H12	119.9
C2—C3—H3	120.6	O1—C13—C12	123.12 (15)
C5—C4—C3	120.35 (17)	O1—C13—C14	115.96 (15)
C5—C4—H4	119.8	C12—C13—C14	120.91 (15)
C3—C4—H4	119.8	O2—C14—C13	118.24 (15)
C4—C5—C6	121.04 (16)	O2—C14—C9	122.79 (15)
C4—C5—H5	119.5	C13—C14—C9	118.97 (15)
F3A—C1A—F1A—F2A	−120.7 (9)	C4—C5—C6—C7	−0.2 (3)
C2—C1A—F1A—F2A	124.4 (7)	C4—C5—C6—N1	179.55 (15)
F3A—C1A—F2A—F1A	120.2 (9)	C8—N1—C6—C5	175.80 (15)
C2—C1A—F2A—F1A	−119.3 (11)	C8—N1—C6—C7	−4.4 (3)
F1A—C1A—C2—C3	36.9 (9)	C3—C2—C7—C6	0.5 (3)
F2A—C1A—C2—C3	158.1 (7)	C1A—C2—C7—C6	179.66 (15)
F3A—C1A—C2—C3	−79.7 (8)	C1—C2—C7—C6	179.66 (15)
F1A—C1A—C2—C7	−142.3 (8)	C5—C6—C7—C2	−0.2 (2)
F2A—C1A—C2—C7	−21.1 (7)	N1—C6—C7—C2	−179.99 (15)
F3A—C1A—C2—C7	101.1 (8)	C6—N1—C8—C9	−179.13 (14)
F1A—C1A—C2—C1	0 (100)	N1—C8—C9—C10	179.02 (15)
F2A—C1A—C2—C1	0 (100)	N1—C8—C9—C14	0.0 (2)
F3A—C1A—C2—C1	0 (38)	C14—C9—C10—C11	0.2 (2)
F3—C1—C2—C3	−129.1 (2)	C8—C9—C10—C11	−178.80 (15)
F1—C1—C2—C3	−3.5 (3)	C9—C10—C11—C12	−0.3 (3)
F2—C1—C2—C3	112.7 (2)	C10—C11—C12—C13	0.3 (2)
F3—C1—C2—C7	51.7 (3)	C11—C12—C13—O1	−179.19 (15)
F1—C1—C2—C7	177.24 (17)	C11—C12—C13—C14	−0.1 (2)
F2—C1—C2—C7	−66.5 (2)	O1—C13—C14—O2	−0.9 (2)
F3—C1—C2—C1A	0 (42)	C12—C13—C14—O2	180.00 (14)
F1—C1—C2—C1A	0 (100)	O1—C13—C14—C9	179.13 (14)
F2—C1—C2—C1A	0 (100)	C12—C13—C14—C9	0.0 (2)
C7—C2—C3—C4	−0.2 (3)	C10—C9—C14—O2	179.97 (15)
C1A—C2—C3—C4	−179.42 (16)	C8—C9—C14—O2	−1.0 (2)
C1—C2—C3—C4	−179.42 (16)	C10—C9—C14—C13	0.0 (2)
C2—C3—C4—C5	−0.2 (3)	C8—C9—C14—C13	178.95 (14)

C3—C4—C5—C6 0.5 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1O \cdots O1 ⁱ	0.84	1.93	2.7510 (15)	165
O2—H2O \cdots N1	0.84	1.81	2.596 (2)	154
C10—H10 \cdots F3 ⁱⁱ	0.95	2.53	3.380 (3)	149
C4—H4 \cdots O1 ⁱⁱⁱ	0.95	2.61	3.392 (2)	140

Symmetry codes: (i) $-x+1/2, y+1/2, -z+1/2$; (ii) $-x+3/2, y+1/2, -z+1/2$; (iii) $-x+1, -y+2, -z+1$.